

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: cedric10

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Bond precision:    C-C = 0.0044 Å                      Wavelength=0.71073

Cell:                      a=8.797(3)              b=12.528(4)              c=18.181(4)  
                                alpha=90              beta=94.30(2)              gamma=90  
Temperature:              293 K

	Calculated	Reported
Volume	1998.1(10)	1998.0(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C16 H15 Fe2 N O5 S3	C16 H15 Fe2 N O5 S3
Sum formula	C16 H15 Fe2 N O5 S3	C16 H15 Fe2 N O5 S3
Mr	509.17	509.20
Dx,g cm-3	1.693	1.693
Z	4	4
Mu (mm-1)	1.792	1.792
F000	1032.0	1032.0
F000'	1036.58	
h,k,lmax	10,14,21	10,14,21
Nref	3528	3517
Tmin,Tmax	0.541,0.650	0.092,0.821
Tmin'	0.483	

Correction method= # Reported T Limits: Tmin=0.092 Tmax=0.821  
AbsCorr = MULTI-SCAN

Data completeness= 0.997                      Theta(max)= 25.000

R(reflections)= 0.0272( 2632)              wR2(reflections)= 0.0660( 3517)

S = 1.047                      Npar= 304

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.



### Alert level C

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C12	--C14	.	6.5 s.u.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				C1 Check
PLAT245_ALERT_2_C	U(iso) H15B	Smaller than U(eq)	C15	by	0.013 Ang**2
PLAT420_ALERT_2_C	D-H Without Acceptor	N31	--H31A	.	Please Check
PLAT742_ALERT_1_C	Angle Calc	112.00(12), Rep	111.98	.....	Missing s.u.
	C11 -S1 -FE1	1.555	1.555	1.555	# 23 Check
PLAT745_ALERT_1_C	D-H Calc	0.86(4), Rep	0.86100	.....	Missing s.u.
	N31 -H31B	1.555	1.555	.....	# 30 Check
PLAT746_ALERT_1_C	H...A Calc	2.42(4), Rep	2.41600	.....	Missing s.u.
	H31B -O3	1.555	1.545	.....	# 30 Check
PLAT747_ALERT_1_C	D...A Calc	3.162(5), Rep	3.16200	.....	Missing s.u.
	N31 -O3	1.555	1.545	.....	# 30 Check



### Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	13 Note
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O4 --C4 . 5.5 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O5 --C5 . 5.3 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 --C1 . 7.5 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 --C2 . 7.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 --C3 . 7.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe2 --C4 . 7.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe2 --C5 . 9.5 s.u.
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2018 Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **ALERT level G** = General information/check it is not something unexpected
- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
11 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### **Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### **Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

